Dynamics of a Two-Level System Coupled to Ohmic Bath: A Perturbation Approach

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Abstract

The physics of a two-level system coupled to Ohmic bath is studied by means of the perturbation approach based on a unitary transformation. Our main results are: The coherence-incoherence transition is at $\alpha_c = \frac{1}{2}[1 + \Delta_r/\omega_c]$; for $\alpha < \alpha_c$ the dynamical quantity $P(t) = \cos(\omega_0 t)\exp(-\gamma t)$; the sussceptibility $\chi''(\omega)/\omega$ is of a double peak structure for $\alpha < \alpha_c$ and the Shiba's relation is exactly satisfied; at the transition point $\alpha = \alpha_c$ the real time correlation function $C(t) \approx -1/\gamma_c^2 t^2$ in the long time limit.

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Studies of the two-level system coupled to Ohmic bath (spin-boson model, SBM) have a long history[1, 2]. Although there were many studies using various kinds of methods, in recent years the physics of SBM has still attracted considerable attention because it provides a universal model for many physical systems[1, 2]. The Hamiltonian of SBM reads

$$H = -\frac{1}{2}\Delta\sigma_x + \sum_k \omega_k b_k^\dagger b_k + \frac{1}{2}\sum_k g_k(b_k^\dagger + b_k)\sigma_z. \tag{1}$$

The notations are the same as usual[1, 2]. In this work we consider the zero bias case with temperature $T = 0$. The Ohmic bath is characterized by its spectral density: $\sum_k g_k^2\delta(\omega - \omega_k) = 2\alpha\omega\theta(\omega_c - \omega)$, where α is the dimensionless coupling constant and $\theta(x)$ is the usual step function.

The Hamiltonian (1) seems to be quite simple. However, it cannot be solved exactly and various approximate analytical and numerical methods have been used[1-13]. Recent studies of SBM focused on its dynamical properties[6-12]. Among these studies, the variational approach proposed by Silbey and Harris[13] is of interest. They proposed to make a unitary transformation: $H' = \exp(S)H\exp(-S)$, with

$$S = \sum_k \frac{g_k}{2\omega_k}\xi_k(b_k^\dagger - b_k)\sigma_z. \tag{2}$$

Then, the variational ground state energy is: $E_g = \langle s_1|\langle\{0_k\}|H'|s_1\rangle|\{0_k\}\rangle$, where $|s_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$ and $|s_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$ are eigenstates of σ_x and $|\{0_k\}\rangle$ is the vacuum state of bosons in which $n_k = 0$ for every k. By minimizing E_g ξ_k is determined as

$$\xi_k \;=\; \omega_k/(\omega_k + \eta\Delta). \tag{3}$$

The authors calculated the renormalized tunnelling Δ_r[13],

$$\eta = \frac{\Delta_r}{\Delta} = \left(e\frac{\Delta}{\omega_c}\right)^{\frac{\alpha}{1-\alpha}} \exp\left[-\frac{\alpha}{1-\alpha}\left(\frac{\eta\Delta}{\omega_c + \eta\Delta} + \ln\frac{\omega_c + \eta\Delta}{\omega_c}\right)\right]. \tag{4}$$

Although the variational method can predict correctly the delocalized-localized transition point $\alpha_l = 1$ at the scaling limit $\Delta/\omega_c \ll 1$, it is not suitable for calculating the dynamical properties of SBM. In this work we present a new analytical approach, based on the unitary transformation ((2) and (3)) and the perturbation theory[14], for

calculating the dynamical preperties of SBM which works well for the coupling constant $0 < \alpha < 1$ and the bare tunnelling $0 < \Delta < \omega_c$. The approach is quite simple and physically clear, and may be easily extended to more complicated coupling systems. Throughout this work we set $\hbar = 1$ and $k_B = 1$.

The unitary transformation (2) can be done to the end and the result is $H' = H'_0 + H'_1 + H'_2$, where

$$H'_0 = -\frac{1}{2}\eta\Delta\sigma_x + \sum_k \omega_k b_k^\dagger b_k - \sum_k \frac{g_k^2}{4\omega_k}\xi_k(2-\xi_k), \tag{5}$$

$$\eta = \exp[-\sum_k \frac{g_k^2}{2\omega_k^2}\xi_k^2], \tag{6}$$

$$H'_1 = \frac{1}{2}\sum_k g_k(1-\xi_k)(b_k^\dagger + b_k)\sigma_z - \frac{1}{2}\eta\Delta i\sigma_y \sum_k \frac{g_k}{\omega_k}\xi_k(b_k^\dagger - b_k), \tag{7}$$

$$H'_2 = -\frac{1}{2}\Delta\sigma_x\left(\cosh\{\sum_k \frac{g_k}{\omega_k}\xi_k(b_k^\dagger - b_k)\} - \eta\right)$$
$$-\frac{1}{2}\Delta i\sigma_y\left(\sinh\{\sum_k \frac{g_k}{\omega_k}\xi_k(b_k^\dagger - b_k)\} - \eta\sum_k \frac{g_k}{\omega_k}\xi_k(b_k^\dagger - b_k)\right). \tag{8}$$

Obviously, H'_0 can be solved exactly because in which the spin and bosons are decoupled. The eigenstate of H'_0 is a direct product, $|s\rangle|\{n_k\}\rangle$, where $|s\rangle$ is $|s_1\rangle$ or $|s_2\rangle$ and $|\{n_k\}\rangle$ means that there are n_k phonons for mode k. The ground state of H'_0 is

$$|g_0\rangle = |s_1\rangle|\{0_k\}\rangle. \tag{9}$$

H'_1 and H'_2 are treated as perturbation and they should be as small as possible. Eq.(3), $\xi_k = \omega_k/(\omega_k + \eta\Delta)$, leads to

$$H'_1 = \frac{1}{2}\eta\Delta\sum_k \frac{g_k}{\omega_k}\xi_k\left[b_k^\dagger(\sigma_z - i\sigma_y) + b_k(\sigma_z + i\sigma_y)\right] \tag{10}$$

and $H'_1|g_0\rangle = 0$. Note that the form of ξ_k, Eq.(3), in this work is determined by $H'_1|g_0\rangle = 0$, instead of minimizing the ground state energy E_g. Thus, we get rid of the variational condition.

The lowest excited states are $|s_2\rangle|\{0_k\}\rangle$ and $|s_1\rangle|1_k\rangle$, where $|1_k\rangle$ is the number state with $n_k = 1$ but $n_{k'} = 0$ for all $k' \neq k$. It's easily to check that $\langle g_0|H'_2|g_0\rangle = 0$ (because of the form of η in Eq.(6)), $\langle\{0_k\}|\langle s_2|H'_2|g_0\rangle = 0$, $\langle 1_k|\langle s_1|H'_2|g_0\rangle = 0$, and

$\langle\{0_k\}|\langle s_2|H_2'|s_1\rangle|1_k\rangle = 0$. Moreover, since $H_1'|g_0\rangle = 0$, we have $\langle\{0_k\}|\langle s_2|H_1'|g_0\rangle = 0$ and $\langle 1_k|\langle s_1|H_1'|g_0\rangle = 0$. Thus, we can diagonalize the lowest excited states of H' as

$$H' = -\frac{1}{2}\eta\Delta|g_0\rangle\langle g_0| + \sum_E E|E\rangle\langle E| + \text{terms with higher excited states.} \quad (11)$$

The diagonalization is through the following transformation[4]:

$$|s_2\rangle|\{0_k\}\rangle = \sum_E x(E)|E\rangle, \quad (12)$$

$$|s_1\rangle|1_k\rangle = \sum_E y_k(E)|E\rangle, \quad (13)$$

$$|E\rangle = \sum_E x(E)|s_2\rangle|\{0_k\}\rangle + \sum_E y_k(E)|s_1\rangle|1_k\rangle, \quad (14)$$

where

$$x(E) = \left[1 + \sum_k \frac{V_k^2}{(E+\eta\Delta/2-\omega_k)^2}\right]^{-1/2}, \quad (15)$$

$$y_k(E) = \frac{V_k}{E+\eta\Delta/2-\omega_k}x(E), \quad (16)$$

with $V_k = \eta\Delta g_k\xi_k/\omega_k$. E's are the diagonalized excitation energy and they are solutions of the equation

$$E - \frac{\eta\Delta}{2} - \sum_k \frac{V_k^2}{E+\eta\Delta/2-\omega_k} = 0. \quad (17)$$

The dynamical quantity $P(t) = \langle b,+1|\langle +1|e^{iHt}\sigma_z e^{-iHt}|+1\rangle|b,+1\rangle$ is defined in Ref.[1], where $|+1\rangle$ is the eigenstate of $\sigma_z = +1$ and $|b,+1\rangle$ is the state of bosons adusted to the state of $\sigma_z = +1$. Because of the unitary transformation ($e^S\sigma_z e^{-S} = \sigma_z$)

$$P(t) = \langle\{0_k\}|\langle +1|e^{iH't}\sigma_z e^{-iH't}|+1\rangle|\{0_k\}\rangle, \quad (18)$$

since $e^S|+1\rangle|b,+1\rangle = |+1\rangle|\{0_k\}\rangle$. Using Eqs.(11)-(17) the result is

$$\begin{aligned}P(t) &= \frac{1}{2}\sum_E x^2(E)\exp[-i(E+\eta\Delta/2)t] + \frac{1}{2}\sum_E x^2(E)\exp[i(E+\eta\Delta/2)t] \\ &= \frac{1}{4\pi i}\oint_C dE' e^{-iE't}\left(E' - \eta\Delta - \sum_k \frac{V_k^2}{E'+i0^+-\omega_k}\right)^{-1} \\ &+ \frac{1}{4\pi i}\oint_C' dE' e^{iE't}\left(E' - \eta\Delta - \sum_k \frac{V_k^2}{E'-i0^+-\omega_k}\right)^{-1},\end{aligned} \quad (19)$$

where a change of the variable $E' = E + \eta\Delta/2$ is made. The real and imaginary parts of $\sum_k V_k^2/(E' \pm i0^+ - \omega_k)$ are denoted as $R(E')$ and $\mp\gamma(E')$,

$$R(\omega) = -2\alpha\frac{(\eta\Delta)^2}{\omega+\eta\Delta}\left\{\frac{\omega_c}{\omega_c+\eta\Delta} - \frac{\omega}{\omega+\eta\Delta}\ln\left[\frac{|\omega|(\omega_c+\eta\Delta)}{\eta\Delta(\omega_c-\omega)}\right]\right\}, \qquad (20)$$

$$\gamma(\omega) = 2\alpha\pi\omega(\eta\Delta)^2/(\omega+\eta\Delta)^2. \qquad (21)$$

The integral in (19) can proceed by calculating the residue of integrand and the result is $P(t) = \cos(\omega_0 t)\exp(-\gamma t)$, where ω_0 is the solution of equation

$$\omega - \eta\Delta - R(\omega) = 0 \qquad (22)$$

and $\gamma = \gamma(\eta\Delta) = \alpha\pi\eta\Delta/2$ (the second order approximation). This $P(t)$ is of the form of damped oscillation and one can check that the solution ω_0 is real when $1 > 2\alpha\omega_c/(\omega_c+\eta\Delta)$. When $1 < 2\alpha\omega_c/(\omega_c+\eta\Delta)$, the solution ω_0 is imaginary and we have an incoherent $P(t)$. $\alpha_c = \frac{1}{2}[1+\eta\Delta/\omega_c]$ determines the critical point where there is a coherent-incoherent transition. Note that when $\Delta/\omega_c \ll 1$, we have $\alpha_c = 1/2$, $\omega_0 = 0$ and $P(t) = \exp(-\gamma_c t)$ ($\gamma_c = \pi e\Delta^2/4\omega_c$ since $\eta = e\Delta/\omega_c$ from Eq.(4)), which is the same as was predicted by previous authors ($\gamma_c = \pi\Delta^2/2\omega_c$ in Ref.[3, 4, 6]). Fig.1 shows the calculated ω_0/Δ_r as functions of α ($\alpha \le \alpha_c$) for $\Delta = 0.01$, 0.1, and 0.5. $\Delta_r = \eta\Delta$ is the renormalized tunnelling. The dotted line is $\gamma/\Delta_r = \alpha\pi/2$.

Since $e^S\sigma_z e^{-S} = \sigma_z$, the retarded Green's function is

$$G(t) \;\; = \;\; -i\theta(t)\left\langle[\exp(iH't)\sigma_z\exp(-iH't), \sigma_z]\right\rangle', \qquad (23)$$

where $\langle ... \rangle'$ means the average with thermodynamic propability $\exp(-\beta H')$. The Fourier transformation of $G(t)$ is denoted as $G(\omega)$, which satisfies an infinite chain of equation of motion[15]. We have made the cutoff approximation for the equation chain at the second order of g_k and the solution at $T = 0$ is

$$G(\omega) = \frac{1}{\omega - \eta\Delta - \sum_k V_k^2/(\omega-\omega_k)} - \frac{1}{\omega+\eta\Delta - \sum_k V_k^2/(\omega+\omega_k)}. \qquad (24)$$

The susceptibility $\chi(\omega) = -G(\omega)$, and its imaginary part is

$$\chi''(\omega) = \frac{\gamma(\omega)\theta(\omega)}{[\omega-\eta\Delta-R(\omega)]^2+\gamma^2(\omega)} - \frac{\gamma(-\omega)\theta(-\omega)}{[\omega+\eta\Delta+R(-\omega)]^2+\gamma^2(-\omega)}. \qquad (25)$$

The $\omega \to 0$ limit of $S(\omega) = \chi''(\omega)/\omega$ is

$$\lim_{\omega\to 0} \frac{\chi''(\omega)}{\omega} = \frac{2\alpha\pi}{(\eta\Delta)^2\{1-2\alpha[1-\eta\Delta/(\omega_c+\eta\Delta)]\}^2}. \tag{26}$$

Besides, the real part of the susceptibility is

$$\chi'(\omega=0) = \frac{2}{\eta\Delta\{1-2\alpha[1-\eta\Delta/(\omega_c+\eta\Delta)]\}}. \tag{27}$$

Thus, the Shiba's relation[3, 7, 9, 12]

$$\lim_{\omega\to 0} \frac{\chi''(\omega)}{\omega} = \frac{\pi}{2}\alpha\chi'(\omega=0)^2 \tag{28}$$

is exactly satisfied. $S(\omega)$ has a double peak structure for $\alpha < \alpha_c$. For $\alpha \geq \alpha_c$ there is only one peak at $\omega = 0$. Fig.2 shows the $S(\omega)$ versus ω relations for fixed $\alpha = 0.3$ and $\Delta = 0.01$, 0.1, and 0.5.

The symmetrized correlation function

$$\begin{aligned}
C(t) &= \frac{1}{2}\mathrm{Tr}\left\{\exp(-\beta H)[\sigma_z(t)\sigma_z + \sigma_z\sigma_z(t)]\right\}/\mathrm{Tr}[\exp(-\beta H)] \\
&= -\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega \coth(\frac{\beta\omega}{2})\mathrm{Im}G(\omega)\exp(-i\omega t) \\
&= \frac{1}{\pi}\int_0^{\infty} d\omega \frac{\gamma(\omega)}{[\omega-\eta\Delta-R(\omega_0)]^2+\gamma^2}\cos(\omega t),
\end{aligned} \tag{29}$$

where ω_0 is the solution of Eq.(22) and $\gamma(\omega)$ in the denominator is approximated by the second order approximation γ. At the scaling limit $\Delta/\omega_c \ll 1$ and the coherence-incoherence transition point $\alpha = 1/2$,

$$C(t) = \int_0^{\infty} d\omega \frac{\omega\cos(\omega t)}{\omega^2+\gamma_c^2}\frac{(\eta\Delta)^2}{(\omega+\eta\Delta)^2}. \tag{30}$$

$C(t)$ decays algebraically in the long-time limit: $C(t) \approx -1/\gamma_c^2 t^2$, which is the same as what was predicted by previous authors.

In summary: The physics of SBM is studied by means of the perturbation approach based on a unitary transformation. Analytical results of the dynamical quantity $P(t)$, the sussceptibility $\chi''(\omega)$ and the real time correlation function $C(t)$ are obtained for both the scaling limit $\Delta_r/\omega_c \ll 1$ and the general finite Δ_r/ω_c case. Our approach is

quite simple, but it can reproduce nearly all results which agree with those of previous authors using various complicated methods. Besides, our approach can be easily extended to other more complicated coupling systems.

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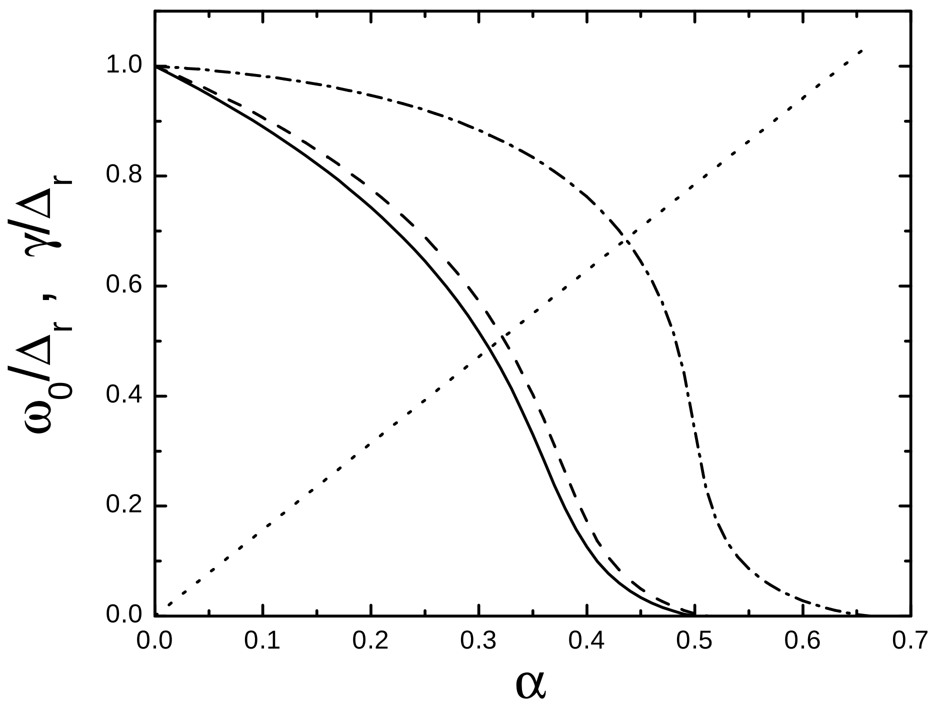
Figure Captions

Fig.1 ω_0/Δ_r versus α relations for $\Delta/\omega_c = 0.01$ (solid line, $\alpha_c = 0.50014$), 0.1 (dashed, $\alpha_c = 0.51212$), and 0.5 (dashed-dotted, $\alpha_c = 0.66244$). The dotted line is $\gamma/\Delta_r = \alpha\pi/2$.

Fig.2 $S(\omega)$ as functions of ω for fixed $\alpha = 0.3$ and $\Delta = 0.01$ (solid line), 0.1 (dashed), and 0.5 (dashed-dotted).



1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
α
ω_0/Δ_r , γ/Δ_r

Fig.1

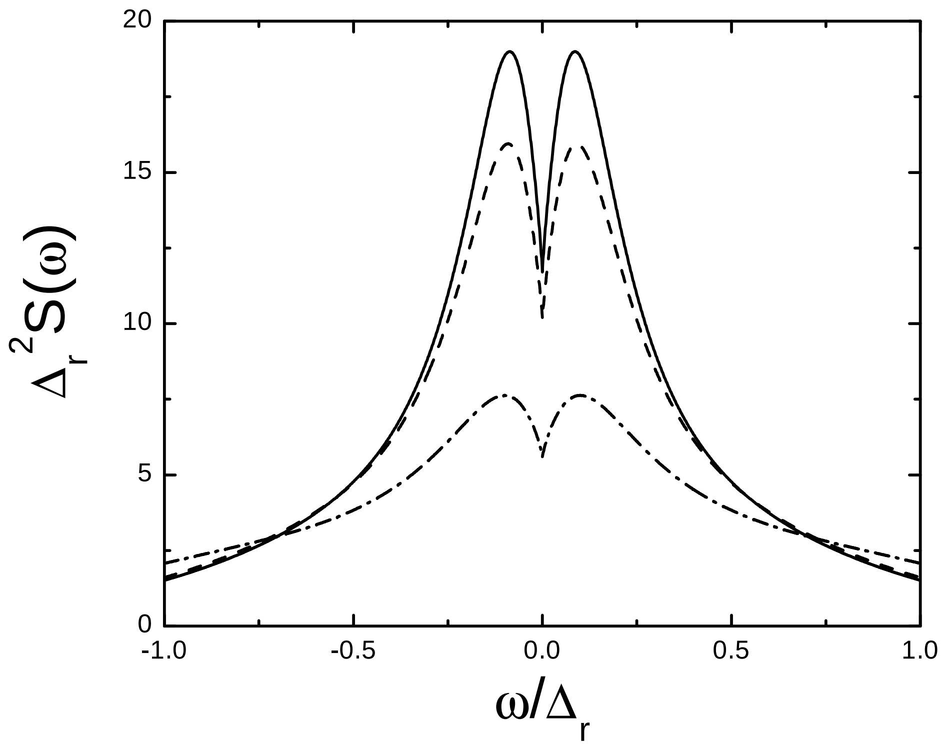


Fig.2